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Relation between structural and optical properties of InN and InxGa1-xN thin films

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Abstract:
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Relation Between Structural and Optical Properties of InN and $In_xGa_{1-x}N$ Thin Films

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Transmission Electron Microscopy (TEM) and optical measurements obtained from InN and $In_{1-x}Ga_xN$ films ($0 < x < 0.54$) grown by Molecular Beam Epitaxy are presented. Energy gaps measured by absorption, PR, and PL for InN films grown on c-plane Al_2O_3 were in the range of 0.7 eV. No In or other inclusions were observed in these films, ruling out the possibility of a strong Mie scattering mechanism. In the $In_{1-x}Ga_xN$ films the relationship between the structural properties and the optical properties, in particular the presence or absence of a Stokes shift between absorption and PL, is discussed. TEM studies show that high quality layers do not have a Stokes shift. Some films had compositional ordering; these films also showed a shift between absorption edge and luminescence peak.

INTRODUCTION

Indium group III-nitride materials are currently under intense investigation mainly due to the controversy in material properties such as the band-gap. The bandgap for InN was originally reported as 1.9 eV [1] but recent optical measurements show that this value is close to 0.7 eV [2]. Earlier grown materials showed however, very high electron densities [3]. Recently grown MBE films have electron densities in the range of $1x10^{18}cm^{-3}$ down to $3x10^{17}$ cm^{-3}. All low electron density materials showed a small bandgap. It has been claimed that In-rich clusters are formed in this material and are responsible for an apparent lower bandap [4]. In-containing nitrides are very important for application in devices but the large size difference between Ga and In atoms can lead to a spinodal decompositions. Both theoretical and experimental evidences were reported [5,6].

In this paper we want to describe the structural and optical quality of the $In_{1-x}Ga_xN$ ($0 < x < 0.54$) grown by Molecular Beam Epitaxy. Transmission Electron Microscopy (TEM), Photoluminescence (PL) and photoabsorption have been used for these studies.

EXPERIMENTAL

Several $In_{1-x}Ga_xN$ with x up to 0.54 samples have been studied. InN film in which low (0.7 eV) bandgaps were measured were evaluated in order to verify the presence or absence of In inclusions. Growth details were described earlier [7].

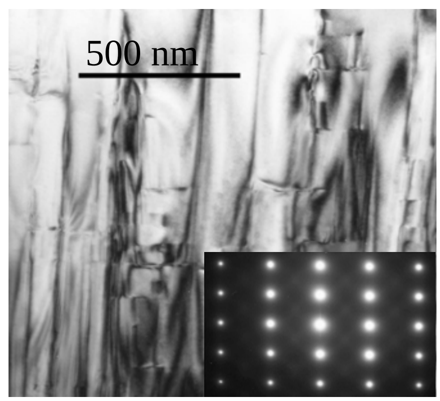

Fig. 1. Bright field image of InN with a small bandgap. Threading dislocations and dislocation loops on c-plane are observed, the inset shows diffraction pattern consistent with InN lattice spacings.

Transmission Electron Microscopy (TEM) studies using classical bright field, high resolution and electron diffraction of InN grown on c-plane indicate that there are no In or other inclusions observed in these films, ruling out the possibility of a strong Mie scattering mechanism (Fig. 1) The observed contrast in the film was uniform and no indication of inclusion was observed. Electron diffraction taken from different areas show only spots consistent with InN (Fig. 1-inset), without any extra spots which would be

characteristic for other phases. Dislocation densities were typically in the mid-10^{10}cm^{-2} range with majority of edge dislocations.

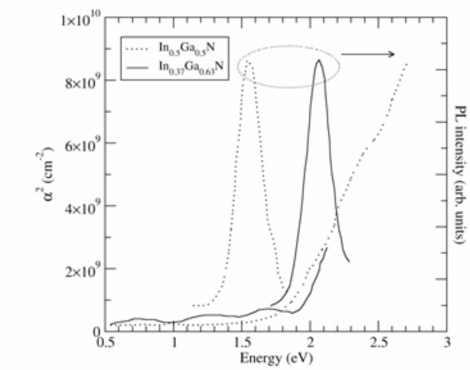

Fig. 2. PL and absorption spectra showing that the "Stokes shift" can be reduced to < 0.1 eV in recently grown high structural quality films (solid lines). The samples with 0.5 eV shift show compositional ordering.

Some samples of the $In_{1-x}Ga_xN$ films grown on thick AlN layer deposited on Al_2O_3 show a Stokes shift (Fig. 2) by about 0.5 eV measured from the absorption edge and room- temperature photoluminescence peak. The samples where this shift is not observed show high structural quality with dislocation density about $6x10^{10}$cm-^{2}.

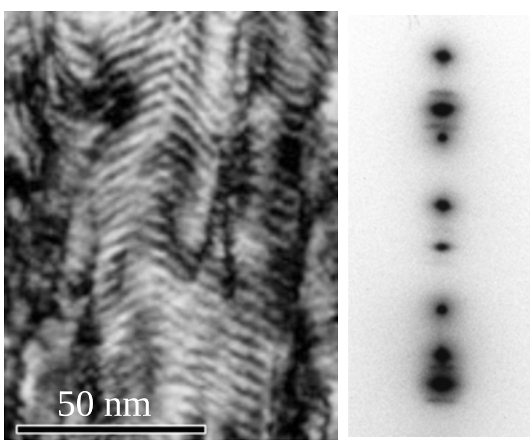

Fig. 3. (a) Bright field image of the $In_{1-x}Ga_xN$ wit x=0.5. Density of dislocations in this layer was estimated ~$1x10^{11}$cm-^{2} Note equally distanced (45Å) fringes due to compositional ordering. (b) Magnified part of the central row of the electron diffraction spots along c-axis (just above the primary beam) showing arrangement of the spots from the Al_2O_3 substrate, AlN buffer layer and the $In_{1-x}Ga_xN$ together with the extra spots forming the arcs around the $In_{1-x}Ga_xN$ spots.

In the samples where this shift was observed (x=0.5) compositional ordering was observed (Fig. 3a). Equally distanced fringes were observed in the entire $In_{1-x}Ga_xN$ film. Electron diffraction (Fig. 3b) show extra spots distributed in a form of small arcs indicating that these fringes do not remain on particular planes but locally very from plane to plane. The distance between these fringes (~45Å) stays approximately constant. The estimated lattice constant of this $In_{1-x}Ga_xN$ layer is a= 3.43Å and c= 5.46Å, indicating composition layer extremely close to this given by the crystal grower (x=0.5).

CONCLUSIONS

In conclusion we can confirm using TEM studies that our InN samples which show low bandgap (~0.7 eV) do not have In inclusions, therefore Mie scattering can be excluded as a mechanism responsible for this low value. For high quality $In_{1-x}Ga_xN$ samples grown by MBE on thick AlN buffer layer the Stokes shift between an absorption edge and photoluminescence was not observed (<0.1 eV). However, for the x=0.5 compositional modulation was observed leading to a Stokes shift, most possible due to two different band edges for InN and GaN driven by strain between the AlN buffer and the $In_{1-x}Ga_xN$.

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